МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Computational Methods of dynamics of classical and quantum systems. Part 8". (Training of PhD students of the specialty: 113 – "Applied mathematics" and others)

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи_____ Хецеліус О.Ю.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
Протокол №1 від 28/08/2021 Зав. кафедри_____ Глушков О.В.

Одеса 2021

THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
ODESSA STATE ENVIRONMENTAL UNIVERSITY

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Computational Methods of dynamics of classical and quantum systems. Part 8". (Training of PhD students of the specialty: 113 – "Applied mathematics" and others)

Odessa 2021

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Computational Methods of dynamics of classical and quantum systems. Part 8”. (Training of PhD students of the specialty: 113 – “Applied mathematics” and others)

Compiler:
Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Editor:
Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

PREFACE

Discipline "Computational methods of dynamics of classical and quantum systems" is a compulsory discipline in the cycle of professional training of postgraduate students (3 level of education) in specialty 113 - Applied mathematics.

It is aimed at assimilating (assuring) a number of planned competences, including developing fundamentally new and to improve the existing modern computational methods and algorithms of quantum mechanics, geometry and electrodynamics for the analysis, modeling and prediction of the properties of classical and quantum systems with pronounced resonance behavior, the ability to analyze data of computer experiments on the study of the characteristics of quantum systems that can be large and require the use of powerful computing resources, the use of modern existing and new advanced computational methods in order to achieve scientific results that create potentially new knowledge in computational mathematics.

The place of discipline in the structural-logical scheme of its teaching: the knowledge gained during the study of this discipline is used in the writing of dissertations, the topics of which are related to the development of new computing methods and algorithms dynamics of complex chaotic systems with possible generalizations on various classes of mathematical, physical and chemical, cybernetic, socio-economic, ecological systems.

The basic concepts of discipline are the fundamental tools of a specialist in the field of applied mathematics.

The purpose of studying the discipline is assimilation (assurance) of a number of competencies, in particular, the achievement of the relevant knowledge, mastering the modern apparatus of quantum geometry and resonance theory, the ability to develop new and improve existing mathematical methods for the analysis, modeling and prediction of spectral properties of quantum systems on the basis of the apparatus of quantum mechanics, geometry and electrodynamics, the search for new resonance phenomena in the dynamics of quantum systems, etc.

After mastering this discipline, the postgraduate student must be able to use modern or personally developed new computing methods, in particular, to analyze, simulate, predict, and program the resonant dynamics of classical and quantum systems with the formulation of appropriate computer experiments

These methodical instructions are for the first-year PhD students and tests performance in the discipline Computational methods of dynamics of classical and quantum systems".

The main topic: Computational methods of modern mechanics, dynamics of quantum systems. Green's function Dirac's equation with nonsingular potential and complex energy

Topic: Computational methods of modern mechanics, dynamics of quantum systems. Green's function Dirac's equation with nonsingular potential and complex energy

Topic: Обчислювальні методи сучасної механіки, динаміки квантових систем. Функція Гріна рівняння Дірака з несингулярним потенціалом та комплексною енергією (ЗБЛ4)

1. Introduction

We present an effective numerical approach to construction of the electron Green function for the Dirac equation with a non-singular central nuclear Fermi-model potential and complex energy. We represent the radial Green function as a combination of two fundamental solutions of the Dirac equation. The approach proposed includes a procedure of generating the relativistic electron functions Ψ with performance of the gauge invariance principle. In order to reach the gauge invariance principle performance we use earlier developed QED perturbation theory approach. In the fourth order of the QED perturbation theory (PT) there are diagrams, whose contribution into imaginary part of radiation width *ImdE* for the multi-electron system accounts for multi-body correlation effects. A minimization of the functional *ImdE* leads to integral- differential Kohn-Sham-like density functional equations. Further check for the gauge principle performance is realized by means of the Ward identities. In the numerical procedure we use the effective algorithm, within which a definition of the Dirac equation fundamental solutions is reduced to solving the single system of the differential equations. This system includes also the differential equations for the Fermi-model nuclear potential and equations for calculating the integrals of the $\iint d\,r_1\, d\,r_2$ type in the Mohr formula for definition of the self-energy shift to atomic levels energies. Such a approach allows to compensate a main source of the errors, connected with numerical integration $\int d\,\xi$ and summation on χ in the Mohr expressions during calculating the self-energy radiative correction to the atomic levels energies.

Different characteristics of the atomic and molecular systems [1-8] can be expressed through the electron and photon Green functions. Usually the energy corrections to levels and oscillation strengths in quantum theory of atoms and molecules are defined by the electron GF with a complex energy parameter *E* and integration on *E* is spread on the indefinite interval. In spectral representation of the electron Green function:

$$G(r_1 r_2 \mid E) = \sum_{n\chi m} \Psi_{n\chi m}(r_2)\Psi_{n\chi m}(r_1)/(E_{n\gamma} - E) \qquad (1)$$

one can separate the partial contributions with fixed value of χ (angular quantum number) (c.f.[5,16-18]). Each partial contribution is presented by multiplying the radial $G(r_1 r_2 | E, \chi)$ the Green function of the radial Dirac equation) and angle parts. Let us remember that, as a rule, the contributions with $|\mathrm{Im}\, E| \le |10 E_0|$ and $|\chi| \le 15$ (here E_0 is the bond energy of the studied state) are important in the modern calculations of the multi-electron systems. The similar expansion for the photon Green function (expansion over the spherical harmonics) separates the radial part – the Green function of the Bessel equation. Usually under calculating the corresponding matrix elements an integration over all angle variables is performed analytically, and integration over the radial variables – numerically.

It is obvious that a development of the effective numerical algorithms for calculating the electron Green function for the Dirac equation with arbitrary potential and complex energy is of great importance for modern relativistic quantum chemistry [1-8]. Our interest to this problem is connected with running calculating the self-energy corrections to atomic levels in the heavy atomic systems and multicharged ions (c.f.[5,9-18,22-26]). Besides, we believe that the similar problem will be arisen in the quantum chemistry of the heavy and super heavy (^{Z}X, Z>100) molecules in some time [5]. In this task all master formulas are conserved, except of the symmetry of the task. It is obvious that the latter in the molecular case differ from the atomic symmetry. From the point of view of the modern quantum calculations of the heavy atoms and multicharged ions it should be mentioned that calculation of the self-energy corrections to the atomic levels energies (radiation widths) have been carried out for low states of the hydrogen-like ions and nuclear charge Z<110 (c.f.[9]). The nuclear finite size correction is usually implemented to the calculation scheme (for example, the relativistic Hartree-Fock or Dirac-Fock methods) by means of using several nuclear models (model of the homogeneous charged sphere, the Gauss model and the Fermi-model) [9-18]. The screening of a nucleus by atomic (molecular) electrons is usually taken into account for within the Dirac-Fock (Dirac-Kohn-Sham) approximations (c.f.[1-21]). By the way, studying the excited heavy and super heavy $(Z \gtrsim 173)$systems with an accurate modelling the nuclear potential (in a whole, nuclear effects in quantum calculations) and accounting for the screening of a nucleus (nuclei) by electrons and radiative effects of the electron shell polarization and probably the Dirac equation non-linear terms [13,14,25,26] remain by very actual problem of the modern theory of multi-electron systems. One could mention here the known difficulties of the modern calculation procedures of quantum chemistry, in particular, in calculating the radiation (self-energy) correction to levels energies of the heavy atomic and molecular systems.

In order to treat correctly a problem of calculating the self-energy correction to atomic (molecular) levels energies in the relativistic quantum chemistry it is

important to have an effective algorithm of calculating the electron Green function for the Dirac equation. As it is well known, the radial electron Green function is presented as a combination of the fundamental solutions of the Dirac equation. One can mention the Whittaker functions as the fundamental solutions of the Dirac equation in a case of the Coulomb potential. As it was noted in refs. [17,18], the known expansions to the Taylor expansion with numerical calculating in the separated blocks are usually used, but there are two significant disadvantages. First of all, calculating the Whittaker function in the separated block increases the dimension of the calculation procedure. Secondly, the corresponding Taylor expansion has a bad convergence for large values of ξ (that is very important for problem (1)) and contains the significant compensations of the separated terms (look more detailed explanation in refs.[17,18]).

Let us remember that following to the Mohr papers [9], within the covariant regularization of the Feynman S-matrix results the self-energy shift to the level energy can be written as follows (c.f. [17,18] too]):

$$E = E_L + E_H(\Lambda) - \frac{1}{\tilde{\alpha}\,\pi\,Z}\left(\frac{3}{2}\ln\Lambda\,\tilde{\alpha}^2 + \frac{3}{8}\right)\langle\beta\rangle, \quad \Lambda\to\infty. \tag{2}$$

and the high-energy part is as follows:

$$E_H(\Lambda) = \mathrm{Re}\,\frac{1}{\pi Z}\int_0^\infty d\xi\left[E(\xi,0) - E(\xi,\Lambda)\right], \tag{3}$$

$$E(\xi,\Lambda) = \iint dr_1 dr_2\,\frac{1}{r_{12}}\exp\left[(E_0 - i\xi)^2 - \Lambda^2\right]^{1/2}\psi^+(r_2)\alpha^\mu G(r_1 r_2)\alpha^\mu\psi(r_1) \tag{4}$$

where $\tilde{\alpha} = \alpha Z$ and $\Psi(r)$ is the wave function – solution of the Dirac equation. Let us note that above presented formula are written in the Coulomb units (in the Coulomb units : 1 C.u. of length = 1 a.u.Z; 1 C.u. of energy = 1 a.u. Z^2).

It is important to note that the energy parameter $E = i\,\xi$ in (3) is purely imaginary one and the Green function is complex. This is a direct motivation of the task we are solving here.

As it has been earlier mentioned [9-14], two last terms in (4) is logarithmically diverged at $\Lambda\to\infty$. In the Mohr's paper [9a] it has been received the important result, connected with understanding the mechanism of their compensations, and the finite expressions without divergences are received. From the other side, this procedure is not obligatorily, especially from the point of view of the numerical calculation. In fact, the numerical compensation of the diverged expressions could result in loss of an accuracy. But, as it is indicated in refs. [16-18] this is not main source of the mistake with taking into account for the weak logarithmic divergence (it is meant that the

acceptable accuracy in calculating E_H no worse than 1%). The main source of mistakes is connected with the numerical integration $\int d\xi$ and summation on χ. Naturally, one can present the exact quantitative estimates on the basis of the concrete calculation allowing the variations of different parameters. Following to ref. [16-18], we calculate the self-energy shift strictly on the basis of the formula ((2)-(4). The Λ- dependent part of the contribution will be presented in the following form: $\Lambda E_H/(\Lambda+a)$, where the parameters E_H, a are empirically defined using two reference points: $\Lambda = 40 \cdot |E_0|$ and $\Lambda = 80 \cdot |E_0|$.

2. Dirac equation with complex energy: Fundamental solutions

The radial Dirac equations can be written as follows (in the Coulomb units):

$$f' = -(\chi+1)f/r - V^- g\tilde{\alpha}; \tag{5}$$

$$g' = (\chi-1)g/r + V^+ f\tilde{\alpha};$$

$$V^{\mp} = V(r) - i\xi \mp \tilde{\alpha}^{-2}; \tag{6}$$

where $V(r)$ is the potential of a nucleus. We are interested by a case when the potential is regular for $r \to 0$. It is easy to show (c.f. [16]) that for such a potential the solutions of two types (regular and non-regular at $r \to 0$) exist for each value of ξ and χ:

for $\chi<0$

$$f \sim r^{|\chi|-1}, \quad g \sim r^{|\chi|}, \quad \tilde{f} \sim r^{-|\chi|}, \quad \tilde{g} \sim r^{-|\chi|-1},$$

for $\chi>0$

$$f \sim r^{|\chi|}, \quad g \sim r^{|\chi|-1}, \quad \tilde{f} \sim r^{-|\chi|-1}, \quad \tilde{g} \sim r^{-|\chi|}. \tag{7}$$

The regular solution (f, g) at $r \to 0$ is simply defined by the condition (6) with the accuracy to a normalization. At the same time the singular solutions are not defined by these conditions .

For large values of $|\chi|$ the functions (7) have a strong degree dependence at $r \to 0$ that is a reason of the known calculational difficulties during the numerical integration of the Dirac equations. At large χ the radial functions F and G vary rapidly at the origin of co-ordinates:

$$F(r), G(r) \approx r^{\gamma-1}$$
$$\gamma = \sqrt{\chi^2 - \alpha^2 z^2}$$

To prevent the integration step becoming too small, as usually (c.f.[23,24]) , it is convenient to introduce the new functions isolating the main power dependence:

$$(F,G) = (f,g)\cdot r^{1-|\chi|}; \quad (\tilde{F},\tilde{G}) = (\tilde{f},\tilde{g})\cdot r^{|\chi|+1}. \tag{8}$$

The Green function is a combination of the Dirac equation modified (the power dependence is separated) fundamental solutions:

$$F' = -(\chi + |\chi|)F/r + V^-\tilde{\alpha}G; \quad G' = (\chi - |\chi|)G/r - V^+\tilde{\alpha}F; \tag{9}$$

$$\tilde{F}' = -(\chi + |\chi|)\tilde{F}/r + V^-\tilde{\alpha}\tilde{G}; \quad \tilde{G}' = (|\chi| + \chi)\tilde{G}/r - V^+\tilde{\alpha}\tilde{F}. \tag{10}$$

The functions (*F*, *G*) represent the first fundamental solution, which is regular for $r \to 0$ and singular for $r \to \infty$. Any combination

$$(\tilde{F}, \tilde{G}) + Cr^{2|\chi|}(F, G)$$

satisfies to above written equations for $(\tilde{F}, \tilde{G})$ and represents singular solution at zero. The right chosen combination $(\hat{F}, \hat{G})$ for the single value of the mixing coefficient C (regular for $r \to \infty$) is second fundamental solution $(\hat{f}, \hat{g})$. Finally, the Green function electron function is a four-component matrice with the functions (*F, G*) and $(\hat{F}, \hat{G})$, which are the Dirac equations solutions with account of the corresponding asymptotic conditions. Further one can get from equations (9)-(10) that for $r \to \infty$ [18]:

$$(F,G) \sim \exp Ar; \ (\hat{F},\hat{G}) \sim \exp(-Ar); \quad A = (\tilde{\alpha}^{-2} + \xi^2\tilde{\alpha}^2)^{1/2}. \tag{11}$$

The exponential power is obviously real (i.e., no oscillations). Let us note that this is specifically for purely imaginary energy parameter *E*. The condition (11) defines the functions $(\hat{F},\hat{G})$. As the bi-linear combinations of the function components (7) are presented in the Green function, it is obvious that only their relative normalization is important. It is defined by the Wronscian condition as follows:

$$W = F\widehat{G} - \widehat{F}G \equiv 1. \qquad (12)$$

T
he electron radial Green function is the four component matrice as follows:

$$G(r_1\, r_2 \mid E, \chi) = \begin{pmatrix} \widehat{F}(r_>)F(r_<) & \widehat{F}(r_>)G(r_<) \\ \widehat{G}(r_>)F(r_<) & \widehat{G}(r_>)G(r_<) \end{pmatrix}, \qquad (13)$$

where $r_>$ $(r_<)$ is more (or less) value of r_1, r_2; the functions (F,G) and $(\widehat{F},\widehat{G})$ satisfy the Dirac equations (8)-(9), their asymptotical conditions (6), (11) and the Wronscian normalization condition. It can be easily shown that exchanging the solution $(\widehat{F},\widehat{G})$ by any combinations $(\widehat{F},\widehat{G}) + B r^{2|\chi|}(F,G)$ does not break the Wronscian condition (c.f.[17,18]).

3. Nuclear potential for the Dirac equation: Fermi model

Earlier we have calculated some characteristics of hydrogen-like and other multi-electron ions with using the nuclear charge distribution in the form of a uniformly charged sphere and Gaussian form (c.f. [16-19,23, 22-24]). The advantage of the Gaussian form nuclear charge distribution is provided by using the smooth function instead of the discontinuous one as in the model of a uniformly charged sphere [22]. It is obvious that it simplifies the calculation procedure and permits to perform a flexible simulation of the real distribution of the charge in a nucleus. In last years to define the nuclear potential it is usually used the Fermi model for the charge distribution in the nucleus $\rho(r)$ (c.f.[9,24]):

$$\rho(r) = \rho_0 / \{1 + \exp[(r - c)/a)]\} \qquad (14)$$

where the parameter *a=0.523* fm, the parameter *c* is chosen by such a way that it is true the following condition for average-squared radius:

$$<r^2>^{1/2} = (0.836 \cdot A^{1/3} + 0.5700)\text{fm}.$$

Further let us present the formulas for the finite size nuclear potential and its derivatives on the nuclear radius. If the point-like nucleus has the central potential *W(R),* then a transition to the finite size nuclear potential is realized by exchanging *W(r)* by the potential [17]:

$$W(r|R) = W(r)\int_0^r dr\, r^2 \rho(r|R) + \int_r^\infty dr\, r^2 W(r)\rho(r|R). \qquad (15)$$

We assume it as some zeroth approximation. Further the derivatives of various characteristics on R are calculated. They describe the interaction of the nucleus with outer electron; this permits recalculation of results, when R varies within reasonable limits. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr' r'^2 \rho\left(r'\middle|R\right) + \int_r^\infty dr' r' \rho\left(r'\middle|R\right) \qquad (16)$$

It is determined by the following system of differential equations [23]:

$$V'nucl(r,R) = \left(1/r^2\right)\int_0^r dr' r'^2 \rho\left(r',R\right) \equiv \left(1/r^2\right) y(r,R)$$
$$y'(r,R) = r^2 \rho(r,R) \qquad (17)$$

$$\rho'(r) = (\rho_0 / a)\exp[(r-c)/a]\{1+\exp[(r-c)/a)]\}^2$$

with the boundary conditions:

$$V_{nucl}(0,R) = -4/(\pi r)$$
$$y(0,R) = 0\,, \qquad (18)$$
$$\rho(0) = \rho_0 /\{1+\exp[-c/a]\}$$

The corresponding system of equations includes the equations for the density distribution function too. The corresponding derivative of potential on the nuclear radius is as follows:

$$\partial W\left(r|R\right)/\partial r = W(r)\int_0^r dr\, r^2 \partial\rho\left(r|R\right)/\partial R + \int_0^\infty dr\, r^2 W(r)\partial\rho(r|R)/\partial r\,, \qquad (19)$$

The derivative of the physical characteristics, corresponding to potential $W(r|R)$, on the nuclear radius is represented by the matrix element:

$$\partial W(R)/\partial R = \int_0^\infty dr\, r^2 \left[F_{nlj}^2(r) + G_{nlj}^2(r)\right]\partial W(r|R)/\partial R \qquad (20)$$

It should be remembered that the nuclear finite size correction is not correctly taken into account within the perturbation theory as a matrix element of two

potentials difference. It is well known that the states functions for two nuclear potentials differ significantly in the important region. Calculation of the potentials, their derivatives, matrix elements is reduced to solving the single system (in fact 1D procedure) of the differential equations (c.f.[16-19,23]).. For example, in order to calculate the potentials $W(r|R)$ and $\partial W(r|R)/\partial R$ the following system of equations should be solved:

$$dW(r \mid R)/dr = P(r \mid R)\, dW(r)/dr ,$$

$$dP(r \mid R) = r^2 \rho(r \mid R) ,$$

$$d[\partial W(r \mid R)/\partial R]/dr = S(r \mid R)\, dW(r)/dr ,$$

$$dS(r \mid R)/dr = r^2 [\partial \rho(r \mid R)/\partial R]$$

with known analytical functions $W(r)$, $\rho(r|R)$. The boundary values at $r \to 0$ are found by expansion to a set on r (c.f.[17,23]).

In refs. [17,18,23] the Dirac equations system is presented and the boundary values of functions (for r =0) for calculating the potential $W(r)$ ($V(r)$) are given. The potential (15), (16) can be expanded to a set on the even degrees:

$$V(r) = V_1 + \sum_{K=2}^{\infty} V_K r^{2K},$$

$$V_1 = -\frac{4\pi}{R}; \quad V_{K>1} = -\frac{4\gamma^{3/2}}{\pi^{1/2}} \cdot \frac{(-\gamma)^{K-2}}{(2K-2)(2k-1)(k-2)!}. \tag{21}$$

Below we also use the complex combinations :

$$V_1^{\pm} = -R\gamma - i\xi \pm \tilde{\alpha}^{-2}.$$

The expansion of the potential to the Taylor set generates the corresponding expansions for the Dirac equations solutions. These conditions are used for the small values r as the boundary values. The first fundamental condition is stable in relation to the little perturbations of the boundary values. So here one could be limited by the first expansion terms:

for $\chi<0$

$$F = 1 + V_1^- \cdot V_1^+ r^2/2(2\chi - 1), \quad G = V_1 r/(2\chi - 1); \tag{22}$$

for $\chi>0$

$$G = -1 + V_1^- \cdot V_1^+ r^2/2(2\chi + 1), \quad F = -V_1 r/(2\chi + 1). \tag{23}$$

The functions $(\hat{F},\hat{G})$ have the following form:

$$\tilde{F}=(f_1+f_2r^2+...)r;\qquad \tilde{G}=g_1+g_2r^2+..., \tag{24}$$

where for $\chi<0$

$$\begin{aligned} &g_1=1, && (2\chi+1)f_1=V_1^-g_1,\\ &-2g_2=V_1^+f_1, && (2\chi+3)f_2=V_1^-g_2+V_2g_1,\\ &-4g_3=V_1^+f_2+V_2f_1, && (2\chi+5)f_3=V_1^-g_3+V_2g_2+V_3g_1, \end{aligned}$$

and for $\chi>0$

$$\tilde{F}=f_1+f_2r^2+....;\qquad \tilde{G}=(g_1+g_2r^2+...)r, \tag{25}$$

$$\begin{aligned} &f_1=1, && (2\chi-1)g_1=V_1^+f_1,\\ &2f_2=V_1^-g_1, && (2\chi-3)g_2=V_1^+f_2+V_2f_1,\\ &4f_3=V_1^-g_2+V_2g_1, && (2\chi-5)g_3=V_1^+f_3+V_2f_2+V_3f_1. \end{aligned}$$

The recurrent procedure allows to calculate any number of terms in the expansions (24), (25).. It is naturally important to define the first χ terms, which are general for all functions $(\tilde{F},G)$. It should be noted that the high power terms in the "right" solution $(\hat{F},\hat{G})$ are defined by the mixture $Cr^{2|\chi|}\ (F,G)$. In order to calculate the mixing coefficient one could use the algorithm [18].

4. Construction of the optimal one-quasi-electron representation

In many calculations of characteristics of the atomic elementary processes it has been shown that an adequate description of these characteristics requires using the optimized basis's of the wave functions. Some time ago Davidson had pointed the principal disadvantages of the traditional representation based on the self-consistent field approach and suggested the optimal "natural orbitals" representation [20]. Nevertheless, there remain insurmountable calculational difficulties in the realization of the Davidson program.

One of the simplified recipes represents, for example, the Kohn-Sham density functional method [21]. Unfortunately, this method doesn't provide a regular refinement procedure in a case of the complicated atomic systems with several quasiparticles (electrons or vacancies above a core of the closed electron shells). Our version of the density functional method, based on the formally exact QED PT, uses some effective bare potential for this purpose [16-19].

In ref. [19] it has been proposed "ab initio" optimization principle for construction of the relativistic orbital basis's. The minimization condition of the gauge dependent multielectron contribution of the lowest QED PT corrections to

the radiation widths of the atomic levels is used. The details of procedure can be found in ref. [19]. Here we briefly describe the key moments. In the fourth order of QED PT there appear diagrams, whose contribution into the ImδE accounts for the exchange-polarization effects. This contribution describes the collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). Let us examine the multi-electron atom with 1QP in the first excited state, connected with the ground state by the electric dipole radiation transition. In the zeroth order of QED PT we use the 1-electron bare potential $V_N(r)+V_C(r)$. The mean field potential $V_C(r)$ is related to the electron density $\rho_C(r)$ in a standard way [16]. Moreover, all the results of the approximate calculations are the functionals of the density $\rho_C(r)$. Further one may treat the lowest order multi-electron effects, in particular, the gauge dependent radiative contribution for a certain class of the photon propagator calibration. This value is considered to the typical electron correlation effect, whose minimization is a reasonable criterion in searching the optimal one-electron basis of PT. All the gauge non-invariant terms are multi-electron by their nature (the particular case of the gauge non-invariance manifestation is the non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the "length" and "velocity" transition operator forms). Quite complicated calculation of contribution of the QED PT fourth order polarization diagrams into Im ΔE gives the following result [19]:

$$Im\ \Delta E_{ninv}\ (\alpha\text{-}s;\ b) = -\ C \int\int\int\int dr_1\, dr_2\, dr_3\, dr_4 \sum_{\substack{n>f \\ m\le f}} \left(\frac{1}{\omega_{mn} + \omega_{\alpha s}} + \frac{1}{\omega_{mn} - \omega_{\alpha s}} \right)$$

$$\psi_\alpha^{+}\ (r_1)\ \psi_m^{+}(r_2)\ \psi_s^{+}\ (r_4)\,\psi_n^{+}(r_3)\,\frac{1-\alpha_1\alpha_2}{r_{12}}\,\{[\ (\alpha_3\alpha_4\ -\ \alpha_3\, n_{34}\ \alpha_4\, n_{34})\ /\ r_{14}\ ]\ \sin\ [\ \omega_{\alpha n}\,(r_{12} + r_{34}\ )]\ +$$

$$\omega_{\alpha n}\ \cos\ [\ \omega_{\alpha n}\,(r_{12} + r_{34}\ )]\ (1+\alpha_3\, n_{34}\ \alpha_4\, n_{34})\}\ \psi_m\ (r_3)\ \psi_\alpha\ (r_4)\ \psi_n\ (r_2)\ \psi_s\ (r_1).$$

(26)

Here, C is a gauge constant, f is the boundary of the closed shells; $n \ge f$ indicating the unoccupied bound and the upper continuum electron states; $m \le f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization). The minimization of the density functional $Im\ \Delta E_{ninv}$ leads to the integral differential equation for the ρ_c, that is numerically solved. In ref. [19] it is developed more simplified calculational procedure. In result one can get the optimal one-electron basis of PT. Below we first use such a basis in calculation of the radiative corrections to atomic levels energies.

5. Procedure for definition the second fundamental solution of the Dirac equation and anti- Wronscian

In ref [17,18] it has been introduced the bi-linear combination, which was called as the anti- Wronscian:

$$W^{-} = F \cdot \hat{G} + \hat{F} \cdot G. \qquad (27)$$

It can be received from the Dirac equation and the Wronscian condition that

$$F \cdot \hat{G} = 1/2 + O(r), \qquad \hat{F} \cdot G = -1/2 + O(r) \quad \text{for } r \to \infty, \qquad (28)$$

where $\hat{F}, \hat{G}$ is the regular solution (9)-(10) at $r \to \infty$. It means that $\hat{W}^{-}$ is the finite function elsewhere and it is right for any energy E (even E>0, when the Dirac equation solutions are oscillating for $r \to \infty$):

$$W^{-} \sim 1/\mathrm{r} \quad \text{for} \quad r \to \infty. \qquad (28)$$

The main advantage for the W^{-} introduction is connected with a simpleness of asymptotes, that is make more simple its integration, analysis of the numerical errors and modelling in the region of the asymptotically large values r. Taking into account the Wronscian condition, one may write as follows :

$$\hat{F} = \left(W^{-} - 1\right)/2G, \qquad G = \left(\hat{W}^{-} + 1\right)/2F, \qquad (29)$$

So, the second fundamental solution can be easily found if the first solution (F, G) and the anti- Wronscian are known. Further, following to ref.[18], one may write the differential equation for function W^{-}:

$$W^{-\prime} = \tilde{\alpha} V^{-}\left(\hat{W}^{-} + 1\right) G/F - \tilde{\alpha} V^{+}\left(W^{-} - 1\right) F/G \qquad (30)$$

with asymptotic conditions :

$$W^{-\prime} \to -W/r \quad \text{for } r \to \infty. \qquad (31)$$

It can be shown that if some function $\tilde{W}^{-}$ satisfies to the equation (30) then any function of the following type

$$\tilde{W}^{-} + C r^{2|\varkappa|} F \cdot G. \qquad (32)$$

satisfies to this equation too. The performance of the condition (31) can be reached by means of the corresponding choice of the complex coefficient C for given (F, G) and $\tilde{W}^{-}$. At the same time as the regular solution of the equation (30) as the regular solution of (9),(10) for $r \to \infty$ can be unstable in relation to

the boundary values (for small r) and can exponentially diverged at $r \to \infty$ because of the little mixture of the second fundamental solution. It is quite possible that a contribution of the diverged mixture can become sufficiently significant in a process of the numerical integration.

Another very important aspect of the problem is a correct output of the integrated functions $(\widehat{F}, \widehat{G})$ and W^- to the asymptotes [18]. An effective procedure for realization rational output has been proposed in ref. [12] and based on using the asymptotical equations for W^-. Really, one may represent W^- in the form :

$$W^-(r) = e^{\varphi(r)}. \tag{33}$$

where $\varphi(r)$ is the complex function. The differential equation for anti-wronscian is as follows :

$$dW^- / d\,r = W^- d\,\varphi / d\,r. \tag{34}$$

$$\varphi' = \tilde{\alpha}\left[V^-(W^- + 1)G^2 - V^+(W^- - 1)F^2\right] / GFW^-. \tag{35}$$

Further in a region of the asymptotically large values r one may transit from the exact equation (30) to the asymptotic equations as follows [17,18]:

$$W^{-\prime} = W^{-\prime}\,\mathrm{Re}\,\varphi' + W^-\tilde{\alpha}\,\mathrm{Im}\left\{\left[V^-(W^- + 1)G^2 - V^+(W^- - 1)FF\right] / GFW^-\right\} \tag{36}$$

with the model function :

$$\mathrm{Re}\,\varphi' = -1/r + \sigma_2 / r^2 + \sigma_3 / r^3. \tag{37}$$

It is important that all solutions of the asymptotic differential equations are stable in relation to the numerical errors of integration and, besides, they satisfy to the condition (30). This is opposite to a behaviour of the exact equations (30) solutions. The constants σ_2, σ_3 are simply connected with 1/r expansion for W^- [18]. A control of quality for the integration is fulfilled on the function $X(r) = W^- W^{-*}$. In a region of the asymptotically large values r it is correct the following chain of inequalities :

$$X'(r) < 0,\ X''(r) > 0,\ X'''(r) < 0,\ X^{IV}(r) > 0,\ X^V < 0... \tag{38}$$

for absolutely exact function $X(r)$. The non-fulfilling these condition can be used for earlier diagnostics of the integration numerical errors and transition to the asymptotical differential equations. More details about above described procedure can be found in refs. [16-18].

6. General scheme of calculation for a three-electron system

Taking into account for the further application of the algorithm in calculation of the radiative corrections to the levels energies of the heavy Li-like multicharged ions let us describe briefly the calculation procedure for three-electron systems. More detailed description of all method is given in refs.[22-24].

One may consider the Dirac-Fock type equations for a three-electron system $1s^2nlj$. Formally they fall into one-electron Dirac equations for the orbitals $1s$ and nlj with the potential:

$$V(r) = 2V(r|1s) + V(r|nlj) + V_{ex}(r) + V(r|R) \qquad (39)$$

$V(r|R)$ includes the electrical and the polarization potentials of a nucleus; the components of the Hartree potential:

$$V(r|i) = \frac{1}{Z}\int d\vec{r}\,'\rho(r|i)/|\vec{r} - \vec{r}\,'| \qquad (40)$$

$\rho(r|i)$ is a distribution of the electron density in the state $|\ i\ >$, V_{ex} is the exchange inter-electron interaction. The main exchange effect will be taken into account if in the equation for the $1s$ orbital we assume

$$V(r) = V(r|1s) + V(r|nlj) \qquad (41)$$

and in the equation for the nlj orbital

$$V(r) = 2V(r|1s) \qquad (42)$$

The rest of the exchange and correlation effects are taken into account for in the first two orders of the PT by the total inter-electron interaction [16-19,22-26]. The used expression for $\rho(r|1s)$ coincides with the precise one for a one-electron relativistic atom with a point nucleus. The finiteness of a nucleus and a presence of the second $1s$ electron are included effectively into the energy E_{1s}. Actually, for determination of the properties of the outer nlj electron one iteration is sufficient. Refinement resulting from second iteration (by evaluations) does not exceed correlation corrections of the higher orders omitted in the present calculation. The relativistic potential of core (the "screening" potential) $2V^{(1)}(r|1s) = V_{scr}$ has correct asymptotic at zero and in the infinity; at $\alpha \to 0$ it changes to an appropriate potential constructed on the basis of the hydrogen-like functions. The other details can be found in the papers [22-24].

7. Calculation results for self-energy shift to atomic levels energies: Li-like ions

We have carried out the calculation of spectra for a number of the Li-like heavy ions with nuclear charge Z=18-100, in particular, Li-like argon and uranium. First of all, let us note that in a concrete calculation transition from exact equations (30) to asymptotical ones (34),(35) is under simultaneous fulfilling four conditions:

$$X' < 0,\ X'' > 0,\ X''' < 0, X^{IV} > 0. \qquad (42)$$

Using the exact equations (25) for large r leads to non-fulfilling the third condition and then first one that is meant the divergence of the function.

The attempt to make more long the chain (42) resulted to sharp increasing of the calculation time and does not provede increasimng accuracy of the result. In figure 1 we present the calculated curves for $X = W^{-}W^{-*}$ in dependence upon r.

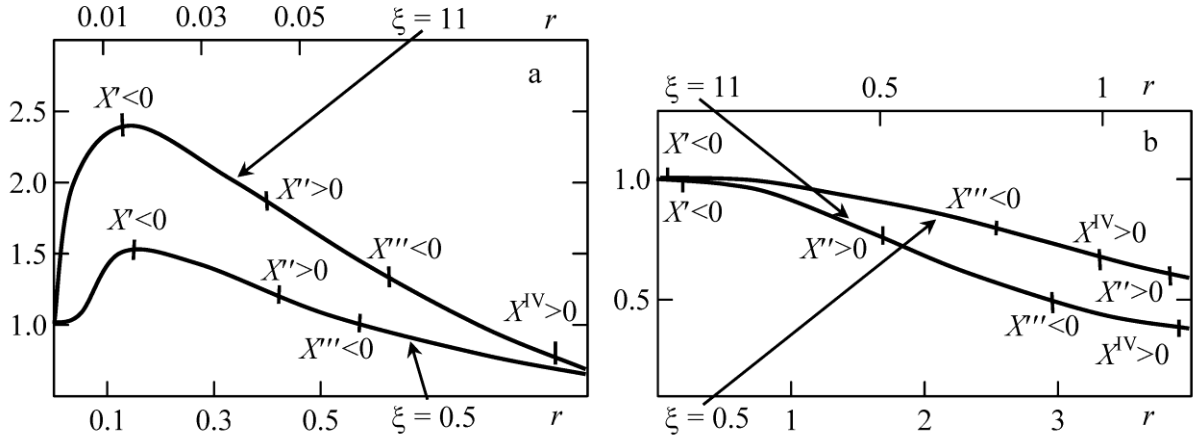

Fig.1. The curves of the $X = W^{-}W^{-*}$ (the Fermi-model is used; nuclear charge $Z_{nucl} = 100$) in dependence upon r : a). χ =-1 ; b). χ =7. The points where the derivatives $X',\ X'',\ X''', X^{IV}$. change a sign, are shown on the curves $X(r)$. The scale of *r* on the x-axe is given for two values ξ.

Below in our calculation we used the Fermi-model nuclear potential and considered the ions with the nuclear charge Z_{nucl}=18, 26, 36 and 92. The points, where the derivatives X', X'', X''', X^{IV} change a sign, are shown on the curves $X(r)$. It is interesting to note that the results obtained are practically identical for the Fermi (present paper) and Gauss [16-18] models of the nuclear charge

distribution. For $\chi = -1$ the behaviour of function after extremum $X(r)$ is not qualitatively dependent upon ξ. For more large values of χ function X'' oscillates. The function X'' reaches the asymptotical value righter than the functions X''', X^{IV} . This is entirely corresponding to the sequence principle (38).

In table 1 we present the experimental (Exp.) and theoretical data for the energies of $2s_{1/2}$-$2p_{1/2}$ transition in spectrum of the Li-like U^{89+}ion, obtained by different methods: E2 - our data (this work) within the QED PT; A – QED PT with the DF zeroth approximation by Shabaev et al; B- multi-configuration Dirac-Fock method by Cheng-Kim-Desclaux; C- relativistic PT on the inter-electron interaction; D – the relativistic many-body PT with zeroth Dirac-Fock potential by Ivanov et al (D) ; E1 –QED PT [22] (look refs. [9,12,15,31-34]). Let us also mention the values of the $2s$-$2p_{1/2}$ transition energy, which are obtained by Persson-Lindgren-Salomonson ($22634 \cdot 10^2 cm^{-1}$) [12] and Blundell ($22650 \cdot 10^2 cm^{-1}$) [35].

Table 1.

Energy (in 10^2 cm^{-1}) of $2s_{1/2}$-$2p_{1/2}$ transition in the spectra of Li-like ions of uranium(see text)

Transition	Exp.	A	B	C	D	E1	E2
$2s_{1/2}$-$2p_{1/2}$	22635 22631	22644	22795	22795	22636	22635	22632
$2p_{1/2}2p_{3/2}$	-	-	336923	336923	336218	336229	336226

In table 2 we present our data for the nuclear finite size effect (NFSE) and self-energy (Lamb shift=LS) contributions to the energy of $2s$-$2p_{1/2}$ transition for the Li-like ions of argon, iron, krypton and uranium. In table 3 we present available experimental data (Exp.) and different calculation results for the energy of the $2s_{1/2}$-$2p_{1/2}$ transition in spectra of the Li-like ions of iron and kripton. The theoretical values are obtained on the basis of different calculation methods: relativistic PT on inter-electron interaction [33]; PT on parameters $1/Z$ and αZ [34], B- multi-configuration Dirac-Fock method [15], the relativistic many-body PT with zeroth Dirac-Fock potential [17] and local Dirac-Fock (and others) potential [31] and QED PT, this paper (see also refs. [22-24]). The corresponding theoretical value of the transition energy for Li-like argon is 25720 (in 10 cm^{-1}); in ref. [31] it is listed the value 25815 cm^{-1} (this is the electron structure value without accounting for the QED corrections).

Table 2

The NFSE and LS contributions (in cm^{-1}) to energy of $2s\text{-}2p_{1/2}$ transition for the Li-like ions with Z=18,26,36,92 (R is an effective nuclear radius; in 10^{-13} cm)

Contribution	Z=18	Z=26	Z=36	Z=92
R	3,15	3,56	3,97	5,42
NFSE	- 10	- 88	- 463	- 267328
-LS	950	3975	12472	333215

Table 3

Energy (in $10\,cm^{-1}$) of $2s_{1/2}\text{-}2p_{1/2}$ transition in the spectra of Li-like ions of iron and krypton (see text)

Ion	Z=26	Z=36
RPT [33]	39158	57628
PT [34]	39335	57628
DF [15]	39335	57628
PT DF [17]	39296	57455
QED DF_L [31]	39199 39604*	57463 58718*
QED, this work	39205	57461
Exp.	39199; 39201	57460; 57463

Note: * the electron structure values without accounting for the QED corrections

Agreement between the theoretical data and experimental results is more or less satisfactory, but the most exact results are presented in refs. [9, 12,22,31]. The calculation has shown that presented generalization of the Ivanov et al approach [17,18,22] to construction of the electron Green function for the Dirac equation with a non-singular nuclear potential and its implementation to the general QED PT formalism [22-24] allows to reach a physically reasonable description of the QED and other contributions to the transition energies, especially, for high-Z ions of the Li-like isoelectronic sequence. In order to check the possibilities of a new approach (within the QED PT [22-24]), we have studied the Li-like ions of argon, iron and krypton. These ions are of the great practical interest for X-ray laser physics etc (look refs. [36-40]). Analyzing the obtained data, in particular, for the Li-like ions of iron and krypton, one could conclude that the approach presented (within the QED PT [22-24]) provides sufficiently high accuracy and physically reasonable description of the corresponding spectra.

8. Tasks for the self-sufficient work

Task Option 1.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**carbon**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 2.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**neon**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 3.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**oxygen**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 4.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**sodium**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 5.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**lithium**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 6.

1). Give the key definitions in theory of optimized one-quaiparticle representatrion of the relativistic perturbation theory with Dirac-Fock equations and Green's function of the Dirac-Fock equation: i) construction of the optimized one-quaiparticle representatrion for Dirac-Fock equations% ii) computing the Dirac-Fock equations; iii) Determination of the Green function of the Dirac-Fock equation; iv) the technical details of the computation code.
2).Explain the key ideas of the numerical approach to construction of the Dirac-Fock optimized representation and realize a concrete scheme for solving of the Dirac-Fock equations and Green's function of the Dirac-Fock equation for concrete atomic system (**magnesium**).
3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

References

1. Khetselius, O.Yu. *Hyperfine structure of atomic spectra;* Astroprint: Odessa, 2008.
2. Glushkov, A.V. *Relativistic Quantum theory. Quantum mechanics of atomic systems*. Astroprint: Odessa; 2008.
3. Svinarenko, A.A. Study of spectra for lanthanides atoms with relativistic many-body perturbation theory: Rydberg resonances. *J. Phys.: Conf. Ser.* 2014, *548,* 012039.
4. Svinarenko, A.A.; Ignatenko, A.V.; Ternovsky, V.B.; Nikola, L.V.; Seredenko, S.S.; Tkach, T.B. Advanced relativistic model potential approach to calculation of radiation transition parameters in spectra of multicharged ions. *J. Phys.: Conf. Ser.* 2014, *548,* 012047.
5. Glushkov, A.V. Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. *In Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology, Series: Progress in Theoretical Chemistry and Physics*; Hotokka, M., Brändas, E., Maruani, J., Delgado-Barrio, G., Eds.; Springer: Cham, 2013; Vol. 27, pp 161–177.
6. Glushkov, A.V.; Ambrosov, S.V.; Ignatenko, A.V.; Korchevsky, D.A. DC strong field stark effect for nonhydrogenic atoms: Consistent quantum mechanical approach. *Int. Journ. Quant. Chem.* 2004, *99,* 936-939.
7. Glushkov, A.V. QED theory of radiation emission and absorption lines for atoms and ions in a strong laser field. *AIP Conf. Proc.* 2008, *1058,* 134-136.
8. Glushkov, A.V.; Loboda, A.V. Calculation of the characteristics of radiative multiphoton absorption and emission lines when an atom interacts with pulsed laser radiation. *J. Appl.Spectr.(Springer).* 2007, *74,* 305-309.
9. Glushkov, A.V.; Malinovskaya, S.V.; Filatov, V.V. S-Matrix formalism calculation of atomic transition probabilities with inclusion of polarization effects. *Sov. Phys. Journal.* 1989, *32(12),* 1010-1014.
10. Dietz, K.; Heβ, B.A. Single particle orbitals for configuration interaction derived from quantum electrodynamics. *Phys. Scripta*. 1989, *39,* 682-688.
11. Glushkov, A.V. Relativistic multiconfiguration time-dependent self-consistent-field theory for molecules. *Sov. Phys. Journal*. 1991, *34*(10), 871-876.
12. Glushkov, A.V.; Efimov, V.A.; Gopchenko, E.D.; Dan'kov, S.V.; Polishchyuk, V.N.; Goloshchak, O.P. Calculation of spectroscopic characteristics of alkali-metal dimers on the basis of a model perturbation theory. *Optika i Spektr.* 1998, *84(5),* 747.
13. Glushkov, A.V.; Malinovskii, A.V.; Efimov, V.A.; Kivganov, A.F.; Khokhlov, V.N.; Vitavetskaya, L.A.; Borovskaya, G.A. Calculation of alkaline metal dimers in terms of model perturbation theory. *J. Struct. Chem.* 1988, *39(2),* 179-185.
14. Glushkov, A.V.; Kondratenko, P.A.; Buyadgi V.V.; Kvasikova, A.S.; Sakun, T.N.; Shakhman, A.S. Spectroscopy of cooperative laser electron-γ-nuclear processes in polyatomic molecules. *J. Phys.: Conf. Ser.* 2014, *548*, 012025.
15. Glushkov, A.V.; Kondratenko, P.A.; Lepikh, Y.I.; Fedchuk, A.P.; Lovett, L.; Svinarenko, A.A. Electrodynamical and quantum-chemical approaches to modeling the electrochemical and catalytic processes on metals, metal alloys, and semiconductors. *Int. Journ. Quant. Chem.* 2009, *109(14),* 3473-3481.
16. *The Fundamentals of Electron Density, Density Matrix and Density Functional*

Theory in Atoms, Molecules and the Solid State, Series: *Progress in Theoretical Chemistry and Physics*. Gidopoulos, N. and Wilson, S., Eds.; Springer: Dordrecht, 2004.
17. Malinovskaya, S.V.; Dubrovskaya, Yu.V.; Vitavetskaya, L.A. Advanced quantum mechanical calculation of the beta decay probabilities. *AIP Conf. Proc*. 2005, *796*, 201-205.
18. Filatov, M.; Cremer, D. A gauge-independent zeroth-order regular approximation to the exact relativistic Hamiltonian—Formulation and applications. *J. Chem. Phys.* 2005, *122*, 044104.
19. Zeng, T.; Fedorov, D.G.; Schnidt, M.W.; Klobukowski M. Two-component natural spinors from two-step spin-orbit coupled wave functions. J. Chem. Phys. 2011, *134*, 214107.
20. Hakel P., Mancini R., Abdalah J. etal. X-ray line polarization spectroscopy of Li-like Si satellite spectra. *J. Phys. B: At. Mol. Phys*. 2009, *42*, 085701.
21. Beiersdorfer, P.; Trabert, E.; Brown, G.V.; Clementson, J.; Thorn, D.B.; Chen, M.H.; Cheng, K.T. Hyperfine Splitting of the 2s1/2 and 2p1/2 Levels in Li- and Be-like Ions of 141Pr. *Phys. Rev. Lett*. 2014, *112*, 233003
22. Ivanova, E.P. Highly efficient tabletop x-ray laser at λ=41.8 nm in Pd-like xenon pumped by optical-field ionization in a cluster jet. *Phys. Rev. A.* 2011, *84*, 043829.
23. Ivanova, E.P.; Grant, I.P. Oscillator strength anomalies in the neon isoelectronic sequence with applications to x-ray laser modeling. *J. Phys.B: At. Mol. Opt. Phys.* 1998, *31*, 2871-2880.
24. Le Bigot, E.O.; Boucard, S.; Covita, D.S.; Gotta, D.; Gruber, A.; Hirtl, A.; Fuhrmann, H.; Indelicato, P.; dos Santos, J.M.F.; Schlesser, S.; Simons, L.M.; Stingelin, L.; Trassinelli, M.; Veloso, J.F.; Wasser, A.; Zmeskal J. High-precision x-ray spectroscopy in few-electron ions. *Phys. Scripta*. 2009, *T134*, 014015.
25. Indelicato, P.; S. Covita, D.S.; Gotta, D.; Gruber, A.; Hirtl, A.; Fuhrmann, H.; Le Bigot, E.O.; Schlesser, S.; dos Santos, J.M.F.; Simons, L.M.; Stingelin, L.; Trassinelli, M.; Veloso, J.F.; Wasser, A.; Zmeskal J. Highly charged ion X-rays from Electron–Cyclotron Resonance Ion Sources. *Nucl. Instr. Meth. in Phys. Res*. A. 2007, *580*, 8-13.
26. Koshelev, K.V.; Labzowsky, L.N.; Tupitsyn, I.I. The interelectron interaction corrections to the hyperfine structure of the $2p_{3/2}$ state in Li-like, B-like and N-like Bi ions. *J. Phys. B: At. Mol. Opt. Phys*. 2004, *37*, 843-851.
27. Pavlov, R.; Mihailov, L.; Velchev, Ch.; Dimitrova-Ivanovich, M.; Stoyanov, Zh.; Chamel, N.; Maruani, J. Effects induced by nuclear deformations and electron correlations on the ground-state energy of low and multiply charged helium like ions in high-temperature plasmas. *J.Phys.: Conf. Ser*. 2010, *253*, 012075
28. Glushkov, A.V.; Malinovskaya, S.V.; Chernyakova Y.G.; Svinarenko, A.A. Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field. *Int. Journ. Quant. Chem.* 2004, *99*, 889-893.
29. Glushkov, A.V.; Malinovskaya, S.V.; Prepelitsa, G.P.; Ignatenko, V.M. Manifestation of the new laser-electron nuclear spectral effects in the thermalized plasma: QED theory of co-operative laser-electron-nuclear processes. *J. Phys.:*

Conf. Ser. 2005, *11*, 199-206.
30. Glushkov, A.V.; Malinovskaya, S.V.; Loboda, A.V.; Shpinareva, I.M.; Gurnitskaya, E.P.; Korchevsky, D.A. Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: calculation of electron-collision strengths and rate coefficients for Ne-like plasma. *J. Phys.: Conf. Ser.* 2005, *11*, 188-198.
31. Glushkov, A.V.; Ambrosov, S.V.; Loboda, A.V.; Gurnitskaya, E.P.; Prepelitsa, G.P. Consistent QED approach to calculation of electron-collision excitation cross sections and strengths: Ne-like ions. *Int. J. Quantum Chem.* 2005, *104*, 562-569.
32. Glushkov, A.V.; Loboda, A.V.; Gurnitskaya, E.P.; Svinarenko, A.A. QED theory of radiation emission and absorption lines for atoms in a strong laser field. *Phys. Scripta.* 2009, *T135*, 014022.
33. Florko, T.A.; Tkach, T.B.; Ambrosov, S.V.; Svinarenko, A.A. Collisional shift of the heavy atoms hyperfine lines in an atmosphere of the inert gas. *J. Phys.: Conf. Ser*. 2012, *397*, 012037.
34. Buyadzhi, V.V. Laser multiphoton spectroscopy of atom embedded in Debye plasmas: multiphoton resonances and transitions. *Photoelectronics*. 2015, *24*, 128-133.
35. Buyadzhi, V.V.; Chernyakova, Yu.G.; Smirnov, A.V.; Tkach, T.B. Electron-collisional spectroscopy of atoms and ions in plasma: Be-like ions. *Photoelectronics*. 2016, *25*, 97-101.
36. Buyadzhi, V.V.; Chernyakova, Yu.G.; Antoshkina, O.A.; Tkach, T.B. Spectroscopy of multicharged ions in plasmas: Oscillator strengths of Be-like ion Fe. *Photoelectronics*. 2017, *26*, 94-102.
37. Khetselius, O.Yu. Relativistic Energy Approach to Cooperative Electron-γ-Nuclear Processes: NEET Effect *In Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics;* Nishikawa, K., Maruani, J., Brändas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, 2012; Vol. 26, pp 217-229.
38. Khetselius, O.Yu. Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. *Int. Journ.Quant.Chem.* 2009, *109*, 3330-3335.
39. Khetselius, O.Yu. Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. *Phys.Scripta.* 2009, *135*, 014023.
40. Khetselius, O.Yu. Optimized Perturbation Theory for Calculating the Hyperfine Line Shift and Broadening of Heavy Atoms in a Buffer Gas. *In Frontiers in Quantum Methods and Applications in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics;* Nascimento, M., Maruani, J., Brändas, E., Delgado-Barrio, G., Eds.; Springer: Cham, 2015; Vol. 29, pp. 55-76.
41. Khetselius, O.Yu. *Quantum structure of electroweak interaction in heavy finite Fermi-systems.* Astroprint: Odessa, 2011.
42. Serot, B.D.; Walecka, J.D. *Advances in Nuclear Physics: The Relativistic Nuclear Many Body Problem*. Plenum Press; New York, 1986.

43. Tomaselli, M.; Schneider, S.M.; Kankeleit, E.; Kuhl, T. Ground-state magnetization of ^{209} Bi in a dynamic-correlation model. *Phys. Rev. C* 1995, *51*, 2989.
44. Nagasawa, T.; Naga, A.; Nakano, M. Hyperfine splitting of hydrogen like atoms based on relativistic mean field theory, *Phys. Rev. C* 2004, *69*, 034322.
45. Glushkov, A.V.; Rusov, V.D.; Ambrosov, S.V.; Loboda, A.V. Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions *In New Projects and New Lines of Research in Nuclear Physics.* Fazio, G., Hanappe, F., Eds.; World Scientific: Singapore, 2003, 126-132.
46. Glushkov, A.V. Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances. *J. Phys.: Conf. Ser*. 2014, *548*, 012021
47. Shahbaz, A.; Muller, C.; Staudt, A.; Burvenich, T.J.; Keitel, C.H. Nuclear Signatures in High-Order Harmonic Generation from Laser-Driven Muonic Atoms. *Phys. Rev. Lett.* 2007, *98*, 263901.
48. Mohr, P.J. Phys. Self-energy of the n = 2 states in a strong Coulomb field. *Phys. Rev. A* 1982, *26*, 2338.
49. Indelicato, P. Relativistic effects in few-electron heavy atoms. Ab initio evaluation of levels energy and transition probabilities. *Phys. Scripta*. 1996, *T65*, 57-62.
50. Blundell, S.A.; Sapirstein, J.; Johnson, W.R. High-accuracy calculation of parity nonconservation in cesium and implications for particle physics. *Phys. Rev. D*. 1992, 45, 1602-1612.
51. Johnson, W.R.; Sapirstein, J.; Blundell, S.A. Atomic structure calculations associated with PNC experiments in atomic cesium. *Phys. Scripta* 1993, *46*, 184.
52. Persson, H.; Lindgren, I.; Salomonson, S.; Lindgren, I. Two-electron Lamb-shift calculations on heliumlike ions. *Phys. Rev. Lett.* 1996, *76*, 204–207.
53. Flambaum, V.V.; Ginges, J.S.M. Radiative potential and calculations of QED radiative corrections to energy levels and electromagnetic amplitudes in many-electron atoms. *Phys. Rev. A* 2005, *72*, 052115.
54. Yerokhin, V.; Artemyev, A.; Shabaev, V.M. QED treatment of electron correlation in Li-like ions. *Phys. Rev. A*. 2007, *75*, 062501.
55. Bieron, J.; Pyykkő, P.; Jonsson, P. Nuclear quadrupole moment of ^{201}Hg. *Phys. Rev. A.* 2005, *71*, 012502.
56. Glushkov, A.V.; Gurnitskaya, E.P.; Loboda, A.V. Advanced Quantum Mechanical Calculation of Superheavy Ions: Energy Levels, Radiation and Finite Nuclear Size Effects. *AIP Conference Proceedings*. 2005, *796*, 217-220.
57. Derevianko, A.; Porsev, S.G. "Dressing" lines and vertices in calculations of matrix elements with the coupled-cluster method and determination of Cs atomic properties. *Phys. Rev. A.* 2005, 71, 032509.
58. Ivanov, L.N.; Ivanova, E.P. Atomic ion energies for Na-like ions by a model potential method *Z* = 25–80. *Atom. Data Nucl. Data Tabl.* 1979, *24*, 95-109.
59. Driker, M.N.; Ivanova, E.P.; Ivanov, L.N.; Shestakov, A.F. Relativistic calculation of spectra of 2-2 transitions in O-and F-like atomic ions. *J.Quant.Spectr. Rad. Transfer.* 1982, *28*, 531-535.
60. Ivanov, L.N.; Ivanova, E.P.; Aglitsky, E.V. Modern trends in the spectroscopy of multicharged ions. *Phys. Rep.* 1988, *166*, 315-390.
61. Ivanova, E.P.; Ivanov, L.N.; Glushkov, A.V.; Kramida, A.E. High order

corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-Like and Ne-Like Ions. *Phys. Scripta* 1985, *32*, 513-522.
62. Ivanova, E.P.; Gulov, A.V. Theoretical investigation of the neon isoelectronic sequence. *Atom. Data Nuc. Data Tabl.* 1991, *49*, 1-64.
63. Ivanov, L.N.; Ivanova, E.P. Method of Sturm orbitals in calculation of physical characteristics of radiation from atoms and ions. *JETP*. 1996, *83*, 258-266.
64. Ivanov, L.N.; Ivanova, E.P.; Knight, L. Energy approach to consistent QED theory for calculation of electron-collision strengths: Ne-like ions. *Phys. Rev. A.* 1993, *48*, 4365-4374.
65. Glushkov, A.V.; Ivanov, L.N.; Ivanova, E.P. Autoionization Phenomena in Atoms. *Moscow University Press*, Moscow, 1986, 58-160
66. Glushkov, A.V.; Ivanov, L.N. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. *Phys. Lett. A* 1992, *170*, 33-36.
67. Glushkov A.V.; Ivanov, L.N. DC strong-field Stark effect: consistent quantum-mechanical approach. *J. Phys. B: At. Mol. Opt. Phys.* 1993, *26*, L379-386.
68. Glushkov, A.V. *Relativistic and Correlation Effects in Spectra of Atomic Systems*. Astroprint: Odessa, 2006.
69. Glushkov, A.V. Relativistic polarization potential of a many-electron atom. *Sov. Phys. Journal.* 1990, *33(1)*, 1-4.
70. Glushkov, A.V. Negative ions of inert gases. *JETP Lett.* 1992, *55*, 97-100.
71. Glushkov, A.V. Energy approach to resonance states of compound superheavy nucleus and EPPP in heavy nuclei collisions *In Low Energy Antiproton Physics;* Grzonka, D., Czyzykiewicz, R., Oelert,W., Rozek, T., Winter, P., Eds.; AIP: New York, *AIP Conf. Proc*. 2005, *796*, 206-210.
72. Glushkov, A.V. Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters *J. Phys.: Conf. Ser.* 2012, *397*, 012011
73. Glushkov, A.V. Advanced Relativistic Energy Approach to Radiative Decay Processes in Multielectron Atoms and Multicharged Ions. *In Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Series: Progress in Theoretical Chemistry and Physics*; Nishikawa, K., Maruani, J., Brandas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, 2012; Vol. 26, pp 231–252.
74. Glushkov, A.V.; Butenko, Yu.V.; Serbov, N.G.; Ambrosov, S.V.; Orlova, V.E.; Orlov, S.V.; Balan, A.K.; Dormostuchenko, G.M. Calculation of the oscillator strengths in Fr-like multiply charged ions. *Journ. of Applied Spectrosc*. 1996, *63(1)*, 28-30.

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Computational Methods of dynamics of classical and quantum systems. Part 8”. (Training of PhD students of the specialty: 113 – “Applied mathematics” and others)

Compiler:
Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Editor:
Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Odessa State Environmental University
65016, Odessa, L’vovskaya str., 15, Room 406 (1st bld.)